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XAFS studies of nickel-doped lead telluride

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ABSTRACT

The problem of impurities and defect states in lead telluride-based semiconductors is of crucial importance for their practical applications. X-ray absorption fine structure (XAFS) techniques are capable to address some of the key issues regarding impurities position, their valent state, as well as the local structural changes of the host lattice in the immediate surrounding of the impurity atoms. In this paper we present the results of the Ni K-absorption edge XAFS studies of Ni-doped PbTe at different temperatures. Analysis of near edge and extended XAFS regions of the measured spectra provided information about exact local environment and lattice ordering around Ni atoms.

1. Introduction

Lead telluride-based semiconductors are extensively used in optoelectronics and thermoelectronics [1–4], and recently also in spintronics and quantum electronics [5,6]. Such a wide range of their application is made possible by their unique properties (tunable direct energy gap, high efficiency of radiative recombination, high values of static dielectric constant, small effective mass of carriers, etc.) and versatile possibilities of their combination. Introduction of a particular dopant atom into the host material can lead to appearance of qualitatively new material properties. Whereas group III impurities induce interesting electronic (pinning of the free carriers concentration and Fermi level) and optical properties (strong plasmon–phonon coupling, activation of local optical modes), transition metals act as magnetic impurities and can provoke interesting effects such as giant magnetoresistance. In the case of a large difference between ionic radii and polarizability of the interchanging ions, impurity atoms are readily displaced from the regular lattice positions, creating that way dipoles whose ordering can lead to ferroelectric phase transitions [7,8]. Although a lot of work has been devoted to study defect states in lead telluride-based semiconductors [7–14] they are not yet fully understood. Most theoretical studies [12,13] assume impurities positioned at ideal lattice sites, which often proved not to be the case. Therefore, it is very important to resolve local structures around impurities in order to better understand their influence on macroscopic characteristics of the materials they are incorporated in.

Element specific X-ray absorption fine structure (XAFS) spectroscopy is at present one of the most powerful tools used for studying structural, electronic and magnetic properties of materials. The near edge region of the absorption spectrum (XANES) is sensitive on electronic structure and contains information on oxidation state and the local coordination geometry around the absorbing atom, whereas the high energy region (EXAFS) is associated with the arrangement of atoms and provides information about the short range order in terms of number, type and distances of atoms in coordination shells and their disorder parameters. Using XAFS spectroscopy we have already resolved the local structures in the series of lead telluride-based semiconductors [15–17]. In this work we extend our studies to Ni-doped PbTe, a semimagnetic semiconductor whose electronic and magnetic properties are not completely understood. Lead telluride crystallizes in rocksalt (NaCl)-type face-centered-cubic (FCC) structure (space group Fm3m, $a = 6.46$ Å), where both Pb and Te atoms are octahedrally coordinated with atoms of different kind. Nickel forms two types of tellurides: (i) antiferromagnetic semiconductor NiTe with a nickel arsenide (NiAs)-type crystal structure (space group $P6_3/mmc$, $a = 3.390$ Å, $c = 5.344$ Å [18]), where Ni occupy a simple cubic lattice which penetrates a close-packed hexagonal Te lattice, and (ii) paramagnetic metallic $NiTe_2$ with a cadmium iodide (CdI_2)-type crystal structure (space group P-3m1, $a = 3.861$, $c = 5.297$ Å [19]), where Te form a hexagonal close packed arrangement while Ni occupy all octahedral sites in alternate layers. Octahedral Te coordination of Ni atoms in both of these tellurides is what provides their partial solubility in PbTe.

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